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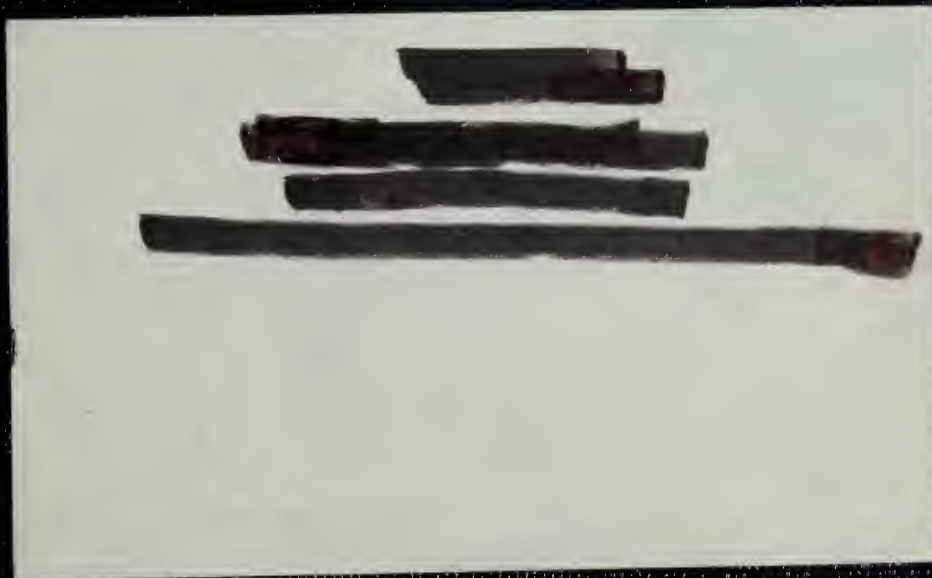
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X-RAY DIFFRACTION PATTERNS FROM FAULTED
FACE-CENTERED
CUBIC AND DIAMOND
CUBIC CRYSTALS

HUGH MILLER DAVIS



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X-RAY DIFFRACTION PATTERNS FROM FAULTED
FACE-CENTERED CUBIC AND DIAMOND CUBIC
CRYSTALS

by

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ABSTRACT

Calculations have been made in an attempt to predict the effects of microscopically fine twinning and of stacking faults on the x-ray diffraction patterns which can be expected from single crystals of materials having the face-centered-cubic or diamond cubic structures. The existence and the effects on x-ray scattering of a coincidence lattice and multiple unit cell in twinned structures are discussed. Additional diffraction peaks are found to appear in diffraction patterns from twinned structures at reciprocal space positions which have non-integer coordinates when referred to the reciprocal lattice of an untwinned crystal. These extra peaks lead to layer line spacings in rotating crystal patterns which are found to be proportional to 3^{-n} where n is the order of the twinning involved.

The extension of methods for determining the effects of random stacking and twinning faults on x-ray diffraction patterns, developed by Paterson and Guentert, is shown to predict non-zero intensities from those planes in faulted diamond crystals which have Miller indices such that $h+k+l = 4n+2$. It is suggested that this provides a partial explanation of the well known "forbidden" reflections from planes of the form $\{222\}$ in crystals having the diamond cubic structure.

The positions and intensities of the $\{222\}$ reflections from a small diamond have been confirmed using a Weissenberg goniometer.

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1. Introduction

The purpose of this investigation has been to determine what changes in x-ray diffraction patterns can be expected when the presence of stacking faults, twins, and other dislocation-related imperfections alter the structure of a perfect crystal, so that it may no longer be mathematically described by one of Bravais lattices. The primary emphasis has been on those structures whose perfect-crystal representations are the face-centered cubic and diamond cubic structures. The methods of approaching the problem which have been developed, however, are capable of being extended to similar problems in crystals having other structures. A particular effort has been made to ascertain whether the "forbidden" reflections from crystals having the diamond cubic structure can be explained on the basis of the presence of imperfections which have altered the arrangement of atoms within the crystal. The determination of the presence of faulted regions having dimensions which are too small to be readily observed with the optical microscope has, in the past, depended chiefly on transmission electron microscopy; however, the necessary thinning of specimens to thicknesses of a few hundred Angstroms may relieve stresses, set up image force conditions, and, in general, greatly disturb the conditions which normally are found in the interior of the crystal. The use of x-rays, on the other hand, allows specimens to be studied which are more nearly three dimensional. If phenomena which have been observed in diffraction patterns and which have not been satisfactorily explained can be correlated with imperfections known to exist within crystals, then the usefulness of x-ray diffraction as a tool for increasing our knowledge of the conditions found on a submicroscopic level within a crystal will have been considerably enhanced. A demonstration that such a dramatic effect as the presence of the "forbidden" reflections is the result of the presence of such imperfections would strengthen the credibility of contentions that the existence of similar faulting in other materials may be determined by x-ray techniques.

Leibovich and Randall studied the x-ray diffraction patterns of single crystals of alpha-iron and aluminum [12, 19]. They reported the existence of extra diffraction peaks, which they attributed to the existence of a coincidence lattice, resulting from the presence of twins in the crystals which they investigated. Hornbeck has also found these extra reflections, and investigated them more fully, using the Buerger precession camera [9]. An effort has been made to develop a theoretical basis on which to evaluate their conclusions.

Before proceeding, it would be well to review the pertinent experimental data and existing theory concerning the presence of the "forbidden" diffraction peaks in crystals having the diamond cubic structure.

The structure factor, F_{hkl} , for the diffraction of waves by a crystalline structure is given by the equation

$$F_{hkl} = \sum_{j=1}^n f \exp [2 \pi i (h u_j + k v_j + l w_j)]$$

where (hkl) are the Miller indices of the plane for which the structure factor is to be determined, f is the scattering factor of each atom, corresponding to the type of radiation being diffracted, and (u_j, v_j, w_j) are the coordinates of the j th atom in the unit cell, n being the number of atoms in the unit cell.

For diamond structures the solutions to this equation indicate that intensity maxima will occur only from those planes for which the Miller indices are either all even or all odd, with the further restriction that when the indices are even their sum must be an integer multiple of four. Hence in diamond, such planes as (222) , (200) , and (420) are now "forbidden" to give diffraction peaks when scattering monochromatic or filtered radiation.

Nevertheless, W. H. Bragg, in 1921, located the diffraction peak from the (222) plane in diffraction patterns of diamond [2]. He had, in fact, been looking for such a maximum, having predicted that it would occur on the basis of the departure of the bonding of carbon from

the spherical symmetry which is assumed in the development of the structure factor equation. That is, the structure factor equation is, in fact, a special case of the Fourier transform of the density of scattering centers within the crystal, with the scattering centers considered to be essentially points so that the integral in the Fourier transform may be replaced by a summation. When the x-rays are scattered by electrons, the assumption of scattering from a point is good only when the major portion of the electron charge cloud surrounding the atoms is in the tightly bound inner shells. In the case of the tetragonal bonding of carbon atoms in diamond, there are four electrons in the inner shells of each atom. The remaining four electrons associated with each atom are distributed throughout the charge clouds defined by the tetragonal bonding orbitals of the structure. It is obvious that there are departures in this arrangement, both from the point concentration of scattering centers and from the spherical symmetry of charge distribution which is implied in this assumption. Whether this departure from the assumptions on which the structure factor calculation is based is sufficient to cause the appearance of the "forbidden" reflections from these crystals has been the subject of much debate in the literature. It should be noted that these (222) peaks have also been reported from germanium and silicon, materials which have the diamond cubic structure [8]. Presumably, the assumption of concentrated scattering power would be more closely met by these materials since the ratio of valence electrons to inner shell electrons is considerably lower than for carbon.¹

The challenges to the asymmetrical charge theory of the "forbidden" reflections can be divided into two principle categories. These may be

¹ Although the Hartree-Fock method for calculating the scattering factor, f , does take into account the wave-functions which describe the distribution of scattering power in each atom of the structure, the computed values of f , once substituted into the summation approximation of the Fourier transform, must, of necessity, act as a point source. The only allowance normally made in the calculations for finite dimensions of the scattering centers is to make a correction for the angle of incidence of the radiation beam.

termed the wave-lattice~~inter~~action theory and the imperfect crystal theory. The assymmetrical charge theory is still by far the most generally accepted and will be discussed first.

Refinements to Bragg's original suggestions have followed the general approach of assuming that the charge distribution in each carbon-carbon bond is more or less concentrated at the center of the bond. This would give a structure much like that of high-cristobalite, with the oxygen atoms which lie midway between each silicon in cristobalite replaced by scattering centers of high electron probability density between each carbon atom in the diamond analog. This approximation is then refined by the assumption of wave-functions which describe such a case, followed by the use of the assumed wave function to calculate the expected intensities from various planes. Order of magnitude agreement with experimental measurements has been obtained with this method [1, 21, 4].

The theories of wave or photon interactions with the lattice are best characterized by several papers by Raman [15, 18]. The contention by Raman that the scattering of x-rays with a change in wave length could account for the "forbidden" reflections, as well as for several other phenomena peculiar to the diamond structure raised such a storm of controversy that an entire issue, (August 29, 1941), of the Proceedings of the Royal Society of London was devoted to a discussion of the problem. Several articles, by many of the most prominent workers in this field, opposed Raman's views, and his theories on this subject never gained acceptance outside of India. A much later paper by Heidenreich partially revived and modified Raman's idea, relating the appearance of the "forbidden" peaks to interactions between the incoming radiation and the Brillouin zone edges [8].

The explanations of the {222} reflections which are based upon the presence of imperfections in the diamond lattice have included suggestions from the workers at the Raman Institute in India that there are regions in the diamond crystals which have octahedral coordination

and, hence a different structure factor, and later papers, also from India, suggesting that the "forbidden" reflections are due to interactions between twinned regions in the crystal and secondary reflections of the incident radiation [17, 6].

Paterson has developed a means of calculating the effects on diffraction patterns of face-centered-cubic crystals when stacking faults and twinning faults are introduced on a single set of parallel close-packed planes [14]. Guentert has extended these calculations so that they are applicable to diamond lattices as well [7]. These calculations, however, have never been extended to the explanation of the existence of the "forbidden" peaks from diamond, and it is the extension of the concepts of Guentert and Paterson which forms the basis for one of the two approaches to the problem discussed in this paper.

A second approach which, at present, provides more information about the extra peaks of Leibovich, Randall, and Hornbeck than it does about diamond has also been developed in the course of the investigation. This approach has been based upon the existence of a coincidence lattice which repeats the lattice points throughout a twinned edifice in a manner similar to the way in which the normal lattice repeats sites in a perfect crystal. The coincidence lattice was first described by Friedel, and has more recently been discussed in some detail by Kohn and Hornstra [5, 11, 10].

The existing experimental data concerning the presence of the "forbidden" peaks in crystals having the diamond symmetry can be summarized as follows:

The reflections from planes of the form $\{222\}$ have been observed from crystals of diamond, silicon, and germanium. These peaks are weak, having intensities on the order of 0.01 to 0.1 those of the strongest peaks recorded [20]. The phenomenon has been recorded both by the diffraction of electrons and of x-rays [8]. According to Lonsdale, only the $\{222\}$ reflections have ever been recorded from natural diamond crystals; however, she states that she has recorded

peaks from other planes for which $h+k+l = 4n+2$ in diffraction patterns of synthetic diamonds manufactured by the General Electric Company [13]. A thorough search of the literature reveals many references to the possibility of the existence of forbidden peaks other than the {222} but no reports of the actual observation of these other peaks has been found.

2. The Coincidence Lattice

One approach to the problem of determining the effects which the introduction of twins or other faults into a perfect crystal will have upon the diffraction of waves by the structure is by the mathematical construction of a coincidence lattice which uniquely defines a relationship between all points in the edifice, both in the faulted regions and in those which remain in the original orientation. Two portions of crystal related to each other by twinning operations alone may easily be described by such a lattice and, as pointed out by Friedel, a quantity known as a twin index may be defined for this lattice [5]. The twin index is simply the ratio of the densities of occupied sites in either of the simple lattices to the density of occupied sites in the coincidence lattice.

The construction of such a coincidence lattice for two face-centered-cubic crystals related to each other by a simple twinning operation may best be understood by referring to figure 1, which is a representation of the (110) plane of a face-centered-cubic crystal. To the left of the heavy line which is the trace of the (111) plane, on which the crystal is twinned, only the lattice sites of the untwinned crystal are shown. These are represented by open circles. To the right of the (111) plane, both the sites of the twinned and the untwinned portions of the edifice are shown. The untwinned sites are represented as before, while those of the twinned portion are shown as filled circles. It will be noticed that certain sites, shown as concentric open and filled circles and joined by dotted lines, are common to both the original lattice and its twin. These are the sites which make up the coincidence

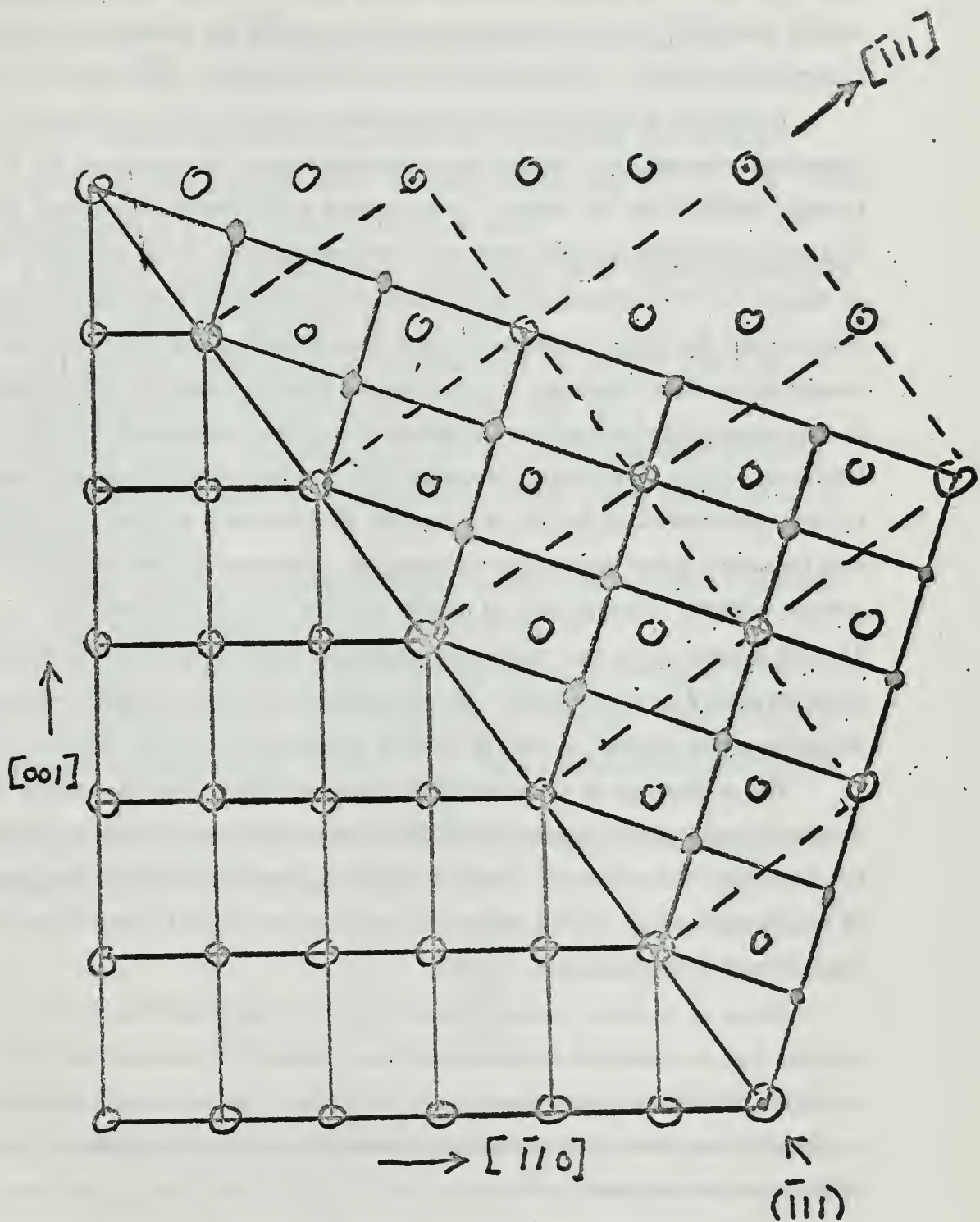


Figure 1. Projection of First Order Twinning Situation on (110) Plane of Reference Crystal, Showing Points of the Coincidence Lattice

lattice. In this case, it will be seen that the separation between sites in the coincidence lattice is three times that of the sites in either of the simple lattices. This relationship holds true for all planes throughout coincidence space. Consequently, the twin index in this case is three.

Using the concept of the coincidence lattice, it is possible to construct a model from which the structure factor calculations for a twinned edifice can be made. The twinned and reference lattices are collapsed together so that they are interpenetrating as in the right half of figure 1. It is then a consequence of the existence of the coincidence lattice that the distance between any two sites having identical surroundings in this structure is three times what it would be when measured in a corresponding direction in either of the two component simple lattices. If the orientation of either the original or the twinned lattice is now considered to be the orientation of the entire edifice, a unit cell can be constructed which has dimensions three times that of the reference lattice. The number of atoms in such a unit cell will be $3^3 \times 2k$ where k is the number of atoms in the unit cell of the reference structure or of its twin. In the case of the face-centered-cubic structure, the number of points in this triple unit cell will be 216.

The existence of this unit cell, having triple the dimensions of a normal unit cell of the structure being studied, will result in the spacing of points in reciprocal space which are one-third that of the spacing of reciprocal space points when the unit cell of normal dimensions is transformed into reciprocal space.

Since it is some representation of the reciprocal lattice of a crystal that is recorded when diffraction studies of its structure are made, this change in the spacing of reciprocal space points should be recorded when the structure of a twinned crystal is investigated by diffraction techniques.

The systematic construction of the triple unit cell and the required structure factor calculations are problems which are readily adaptable to digital computer methods.

The structure factor of such a triple unit cell is computed from the equation

$$F_{hkl} = \sum_{j=1}^{216} f_x \exp [2 \pi i (hu_j + lv_j + lw_j)]$$

where f_x is the x-ray scattering factor for each atom in the cell; (hkl) are the Miller indices of the desired plane; and (u_j, v_j, w_j) are the coordinates of the jth atom in the unit cell.

A computer program written in conjunction with this investigation performs the following sequence of operations.

(1) A set of coordinates is assumed and an integer value is assigned to the lattice parameter of a normal unit cell.

(2) The computer generates all points in the reference lattice which lie within a volume of a cube having edges equal to five lattice parameters in length.

(3) The origin is translated along the [111] direction a distance equal to the lattice parameter multiplied by $\sqrt{3}$.

(4) Points in the twin lattice are generated by rotating the entire block of points by $\pm 60^\circ$, or 180° about the (111) axis. This operation is performed by forming the vector $\begin{bmatrix} u_j \\ v_j \\ w_j \end{bmatrix}$ from the coordinates of each of the points in the reference lattice and multiplying each set of coordinates in turn by a matrix of the form

$$\frac{1}{3} \begin{bmatrix} 2 & 2 & -1 \\ 2 & -1 & 2 \\ -1 & 2 & 2 \end{bmatrix}$$

to obtain the coordinates of the corresponding points in the twinned lattice. It should be noted that by altering the positions of the rows and columns in the three by three matrix and by changing the signs of the terms, rotations of $\pm 120^\circ$, $\pm 60^\circ$, or 180° can be made about any of the axes of the form $\langle 111 \rangle$.

(5) The points generated for the reference crystal and those of

the twin are then examined by computer logic statements, and those which have any coordinate less than zero or greater than or equal to three times the assumed lattice parameter are discarded. The points that remain are those that lie within the triple unit cell.

(6) Finally the computer performs the indicated summation for a set of desired planes and prints the computed structure factor and the square of its absolute value, to which the intensity of the peak is directly related, for each plane.

The rotations of $\pm 120^\circ$ referred to above are not of interest when all atoms in the structure are identical, because such a rotation simply returns the lattice to an orientation which is identical to the original. However, when there is an ordering parameter associated with the structure, such rotations can produce anti-phase domains, or "para-twins", to use a more descriptive term, preferred by the workers at the Naval Postgraduate School.

The solutions generated by this program are in agreement with the previous deduction that there should be points in reciprocal space, and hence in diffraction patterns, which have spacings which are one-third those expected when the diffraction takes place in a perfect crystal.

In order to have the correct inter-planar spacings, the Miller indices of planes which are referred to the triple unit cell must be three times what they would be if referred to the normal unit cell. Table 1 shows calculated structure factors for various planes in the twinned edifice. Only those planes for which the structure factor is non-zero are listed. These planes with non-zero structure factors can be separated into three groups. Those for which the structure factor is 108 and the Miller indices are all integer multiples of three are the normal reflections which would be expected from a crystal which had no twinned portions. The planes which have structure factors of 108 and which have Miller indices which are not integer multiples of three are the peaks due to the presence of the triple unit cell. The

TABLE 1. STRUCTURE FACTORS FOR DIFFRACTION PEAKS FROM FIRST

ORDER TWINS	
Miller Indices of Peaks (Referred to Triple Unit Cell)	Structure Factor
(006)	108
(060)	108
(066)	216
(177)	108
(228)	108
(282)	108
(333)	216
(339)	108
(393)	108
(399)	108
(4 10 10)	108
(600)	108
(606)	108
(660)	108
(717)	108
(771)	108
(822)	108
(933)	108
(939)	108
(993)	108
(999)	216
(10 4 10)	108
(10 10 4)	108
(0 0 12)	108
(0 0 18)	216
(0 6 12)	216
(0 6 18)	108
(1 1 13)	108
(2 8 20)	108

TABLE 1. (Cont'd)

Miller Indices of Peaks (Referred to Triple Unit Cell)	Structure Factor
(3 3 15)	108
(3 9 15)	216
(4 4 16)	108
(5 5 11)	108
(6 0 12)	216
(6 0 18)	108
(6 6 12)	108
(6 6 18)	108
(7 7 19)	108
(8 2 20)	108
(8 8 14)	108
(9 3 15)	216
(9 9 15)	108
(10 4 10)	108
(0 12 12)	108
(0 12 18)	108
(0 18 12)	108
(0 18 18)	216
(1 13 19)	108
(1 19 13)	108
(2 14 14)	108
(3 15 15)	108
(4 10 10)	108
(5 17 17)	108
(6 12 12)	108
(6 12 18)	108
(6 12 18)	216
(6 18 18)	108
(7 13 13)	108

TABLE 1. (Cont'd)

Miller Indices of Peaks (Referred to Triple Unit Cell)	Structure Factor
(8 20 20)	108
(9 15 15)	108
(10 16 16)	108

third group of planes has structure factors of 216. This group consists of those planes for which constructive interference occurs between the reflections from the reference crystal and that of the twin.

If the indices of a plane are squared and then summed, the sum is a measure of the distance between adjacent planes of the same indices, since

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}},$$

where d_{hkl} is the distance between planes having the Miller indices (hkl), and a is the lattice parameter of the crystal.

In Table 1, it will be noticed that for every $h^2+k^2+l^2$ for a reflection which has indices not divisible by three, some plane in the group whose indices are multiples of three has an equal sum. For example, the sum of the squares of the indices of the plane (771) is equal to the similar sum for the plane (339). The significance of this is that it reveals that the "extra" reflections are simply the usual reflections from the twinned portion of the edifice, referred to the reference set of coordinates. Those planes having structure factors of 216 are those for which the plane in the twin, when referred to the reference axes has either the same Miller indices or at least the same combination of indices. For instance, the (531) plane in the twin is parallel to the (135) plane in the reference crystal. Note that these are normal, not triple unit cell coordinates. It is also worth noting that this constructive interference condition occurs only when the sum of the indices is $3n$, n an integer.

Somewhat more complex situations may arise when a crystal, I, twins about a $\langle 111 \rangle$ axis to form a second individual, II, and a third individual is now created by a similar rotation about a non-parallel $\langle 111 \rangle$ axis of I. The third individual, III, will be in twinned orientation with both I and II, but the coincidence lattice which relates sites in III to those in II will have a twin index of nine instead of three. Such a process can continue to repeat by the formation of additional twin

related individuals by successive twinning about the $\langle 111 \rangle$ axes of newly created twins. When this takes place the twin indices for the coincidence lattices which relate the points in the various individuals making up the edifice will increase according to the sequence 3, 9, 27, 3^n , where n is called the order of the twin. In the example given above II and III are in first order relation to I, but are in second order relation to each other. It follows from the above discussion that the unit cell for the calculation of structure factors from second order twins will have dimensions of nine times the lattice parameter, while for third order twins the dimensions will be 27 times those for the normal unit cell.

In general, the number of atoms in a multiple unit cell will be given by the equation

$$N = (3^m)^3 \times 2k,$$

where N is the number of atoms in the multiple unit cell, m is the order of the twin, and k is the number of atoms in the single unit cell.

Since the specification of the coordinates of each atom requires three integers, the storage capacity of even the largest digital computer is soon saturated as m becomes larger.

For second order twins in a face-centered-cubic structure, however, $N = 5832$, a number which is well within the capacity of the CDC 1604 computer. It should also be realized that in an edifice consisting of a large number of individuals, all in twinned relation to each other, there will almost certainly be regions in which higher order twins adjoin each other at what has been called a "twin-join" by Kohn [11]. As Hornstra and Kohn have pointed out, the energy of such a boundary is proportional to the twin index [10, 11]. From these considerations, it appears that the order of twinning in a heavily twinned edifice may be limited to fairly small values, if fracture is not to occur. If this is indeed the case, it would not be necessary to compute solutions for twins of orders greater than three or four.

A compilation of structure factors for an edifice modelled after

the explanation of second order twinning given above has been made. There are three individuals in the edifice, two of which are in first order relation to the reference and in second order relation to each other. In this case the reflections which would occur from an untwinned structure are those which have indices which are multiples of nine.

Table 1 and the corresponding data for ~~second order twinning~~ are in partial qualitative agreement with the experimental observations of Hornbeck and Randall [9, 19].

That is, they predict the existence of x-ray diffraction peaks which would not be found in the diffraction patterns of untwinned crystals. Furthermore, the position of these peaks at spacings equal to multiples of one-third or one-ninth of their usual spacing also appears to agree with the observed data. The predicted intensities of the extra peaks, however, are equal to those which would be expected from an untwinned crystal, while the experimental extra reflections are quite weak. Furthermore, the number of extra peaks observed is much smaller than the number predicted.

No completely satisfactory explanation of these discrepancies has been developed, but at least two possible reasons for the disagreement can be suggested.

If it is assumed that the portion of the crystal examined is, in fact, composed of a large number of crystallites which are all in twinned orientation to each other, it may be possible that the average effect of these many randomly, but discretely oriented individuals is mimetic. That is the diffraction pattern of the edifice mimics the diffraction pattern of a single individual. Friedel has mentioned the possibility of such effects [5]. In this case the few faint reflections from the multiple unit cell would result from a departure from complete randomness in some portion of the volume illuminated by the x-ray beam.

The second suggested explanation for the disagreement between the calculations and the observed results simply assumes that the major portion of the volume of crystal illuminated by the x-ray beam is

in the assumed orientation, but that there are small regions which are in twin orientation with respect to the rest of the volume. The relative intensities of the peaks from the various orientations would be a function of the number of atoms in the different orientations. Twins of small volume would be expected to produce much smaller peaks than the portion of the crystal which is in the assumed orientation and contains a large majority of the atoms illuminated.

The program described above has also been used to determine the effects of fine twinning on the diffraction patterns of crystals having the diamond structure. The results are in every way analogous to those presented above. The use of this program as now constructed does not give any indication that the forbidden reflections are due to twinning. This method is, of course, an oversimplification of the conditions which actually exist in faulted crystals. A method which overcomes some of the artificialities of this approach will be discussed in the next section.

3. A Statistical Approach

As mentioned at the end of the previous section, the geometrical approach to the problem of calculating the effects of twinning and other faults on the structure factor of a crystalline edifice is a great oversimplification, and does not present a sufficiently accurate approximation to the actual conditions that exist to give anything but very crude qualitative results.

Among the problems ignored in constructing the models of the previous section were the effects of the sizes of the individual twins within the edifice, the possibility of the existence of other types of faults, and the effect that the location of the composition plane of the twin has upon the actual positions of the scattering centers within the edifice.

The normal stacking sequence of parallel close packed planes in face-centered-cubic crystals can be described by the sequence ABCABCABCABC..... That is, the atoms in the B layers lie above one

set of hollows formed by the close packing of atoms in the A layers while the atoms in the C layers lie above the other set of hollows. A fault occurs when this sequence is disturbed in some way. The sequence, ABCABCAB(A)CBACBACB..., is an example of the effect of such a fault on the stacking sequence. In this case the fault completely reverses the stacking sequence and results in a twin. Such a fault will be called a twinning fault, or following Paterson, a growth fault [14]. A stacking or deformation fault, on the other hand, simply interrupts the stacking sequence which is already established in the crystal. The sequence ABCABCAB(A)BCABCABC.... contains such a fault. It can be seen that the positions of the atoms in layers above the first fault in such a faulted structure will depend upon both the frequency of occurrence of faults and the exact plane upon which each fault appears.

If the distribution of faults on each set of close packed planes is statistically random, the construction of an unit cell to describe the position of every atom in the edifice becomes impossible using the approach of the last section. Paterson has partially overcome this difficulty by developing a statistical solution for the effects of faults distributed randomly on a single set of parallel close packed planes in face-centered-cubic crystals [14].

A very brief outline of the method used by Paterson is given below. For the details, the reader is referred to the original paper, referenced above.

The basic approach of Paterson is to refer the coordinates of each atom to a new set of hexagonal axes, and then to let each atom be considered an unit cell. If the structure factors of each unit cell in an edifice are known, the intensity of each peak may be calculated by use of the equation

$$I_{hkl} = \sum_j \sum_{j'} F_j F_{j'}^* \exp [2 \pi i / \lambda (\vec{S} - \vec{S}_0) \cdot (\vec{r}_j - \vec{r}_{j'})]$$

where I_{hkl} is the intensity of the diffraction peak from plane (hkl);

F_j and F_j^* are the structure factor of the j th unit cell and the complex conjugate of the structure factor of the j 'th unit cell, respectively;

$\frac{(\vec{S} - \vec{S}_0)}{\lambda}$ is an unit vector defining the direction of the incident radiation; and $(\vec{r}_j - \vec{r}_{j'})$ is the vector from the j 'th unit cell to the j th unit cell.

If the probability of a fault occurring on a given close packed plane is known, and if faulting is assumed to take place on only one set of parallel close packed planes, then a mean value for the product of the structure factors of two unit cells $m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3$ apart can be calculated. Since there is no change in the arrangement of atoms on a given plane, it is found that this mean value, J_m , depends only upon the separation of the unit cells along the \vec{a}_3 direction. In the hexagonal coordinates being used this is the direction perpendicular to the close packed planes. The intensity equation then becomes

$$I = C \sum_{m_3} J_{m_3} \exp \frac{(2 \pi i h_3)}{3}$$

where C is a constant; and h_3 is a continuous variable in the \vec{h}_3 direction in the reciprocal space which corresponds to the hexagonal system chosen. The three in the denominator of the exponential term arises from the fact that the usual unit cell in hexagonal coordinates is three layers high. J_{m_3} can be found in terms of the probability of the occurrence of a fault on a given plane, since from this the probability of a layer a distance m_3 from the reference layer being in either the A, B, or C configurations can be found. Paterson has derived and solved the equations which result from this line of reasoning, and has shown that the results will be a broadening and slight shifting of the locations of certain intensity peaks in reciprocal space.

These results can be summarized as follows:

For those planes that have Miller indice (HK · L) in hexagonal coordinates such that $H - K = 3N$ and $L = 3N'$, where N and N' are integers, there will be sharp peaks with no shifts or broadening, no matter what the

probability of faults may be. The shapes and positions of the peaks from other planes depend upon whether the faults introduced are growth or deformation faults. For deformation faulting with the probability of faulting approaching zero, the other peaks that appear will be sharp and will be from planes having $H - K = 3N - 1$, $L = 3(N' + 1) - 1$; or $H - K = 3N + 1$, $L = 3N + 1$. As the probability of faulting increases, the planes for which $H - K$ and L are not integer multiples of three will begin to broaden and shift toward the reciprocal space points for which $h_3 = 3N + 3/2$. The reciprocal space coordinates of the peaks must now be specified as $(HK \cdot h_3)$, since the coordinate along the \vec{b}_3 direction is no longer an integer. As the peaks broaden and shift, there will be a corresponding decrease in the intensity.

The results from the introduction of growth faults will be similar, but in this case, as soon as a single fault is present, additional peaks will appear at reciprocal space coordinates for which $H - K = 3N - 1$, $L = 3N' + 1$; or $H - K = 3N + 1$, $L = 3(N' + 1) - 1$. These new peaks correspond to those which were shown to result from the presence of first order twins in the previous section. The addition of more twinning faults, i.e., an increase in the probability of twin faults will cause the original set of peaks and those resulting from the presence of twins to broaden and shift toward each other in reciprocal space.

The equations which quantitatively describe the broadening and shifting of peaks as a function of the probability of faults will not be listed here as they are quite involved and are readily available, to those interested, in Paterson's original work [14]. A digital computer solution which solves for the magnitude of the shift along \vec{b}_3 and the peak amplitude as a function of the fault probability has been written in the course of this investigation, and reduces the computations to manageable proportions.

Guentert has shown that the calculations of Paterson for face-centered-cubic materials can be quite easily extended to apply to crystals having the diamond structure [7].

The stacking of planes in a diamond cubic structure is completely analogous to that in face-centered-cubic crystals, except that for every close packed layer of atoms in the face-centered-cubic structure there is a double layer of atoms in the diamond structure. These double layers consist of atoms bound together at a distance of $\frac{1}{4}\sqrt{3}$ times the cube edge and with the axis of the bond perpendicular to the set of parallel close packed planes being considered.

Such an arrangement can be represented by the sequence AA'BB'CC'AA'BB'.... Assuming with Guentert that the bond angles and distances must be preserved when faults are introduced requires that each double layer, AA'BB', etc., remain intact. Faults may then be introduced only by changing the sequence of double layers. This is precisely the mechanism for the introduction of faults used in Paterson's model.

Guentert points out that the calculations of Paterson amount to the calculation of the structure factor of each layer, considered as an unit cell, and then summing over an infinite sequence of parallel planes. It should be possible, then, to calculate a similar structure factor for a double layer and to apply this directly to Paterson's results.

Representing the double layer by two atoms, one at hexagonal coordinates (0, 0, 0) and the other at coordinates (0, 0, $\frac{1}{4}$), the structure factor of the layer is

$$\begin{aligned} F_{\text{HKL}} &= f \{ \exp[2 \pi i(0+0+0)] \} + f \{ \exp[2 \pi i(0+0+\frac{1}{4}L)] \} \\ &= f [1 + \exp(\frac{\pi i L}{2})] \end{aligned}$$

However, if there are faults in the structure, Paterson's treatment requires that some of the peaks be shifted along the \vec{b}_3 direction, and the integer, L, must be replaced by the continuous variable h_3 . The equation then becomes

$$F_{\text{HK} \cdot h_3} = f a [1 + \exp \frac{\pi i h_3}{2}]$$

Guentert assumes that the difference between h_3 and L will always be very much less than one and that, since the intensity equation is very insensitive to small changes in the argument of the exponential term, L may be retained as the variable. In the development below, however, the effect of small shifts in the peak coordinates has been considered and will be shown to predict intensities for the planes of the form $\{222\}$ which are in order of magnitude agreement with the experimentally reported values.

If the intensity of a reflection from a faulted face-centered-crystal is $I_{\text{fcc}} = f a^2 I_1$ where $f a$ is the x-ray scattering factor of each atom and I_1 is the intensity calculated by Paterson's method, then the structure factor of a faulted diamond is

$$I_{\text{DIAMOND}} = f a^2 \left[1 + \exp \frac{\pi i}{2} (h_3) \right] I_1$$

This reduces to

$$I_{\text{DIAMOND}} = 2 \left(1 + \cos \frac{\pi h_3}{2} \right) I_{\text{fcc}}$$

If the small shifts in h_3 which will occur for faulted crystals are ignored, the planes for which the value of h_3 , or L , since it is then an integer, are equal to odd multiples of two will have extinct reflections. The index, L , in hexagonal coordinates is equivalent to the sum of the Miller indices, $h+k+l$, in cubic coordinates. Having L an odd multiple of two is, then, exactly analogous to the extinction rule in diamond, $h+k+l = 4n+2$. If, however, the small shifts in h_3 predicted by Paterson are allowed, the reflections from these planes will be small but not extinct. If Paterson's equation for structures containing stacking faults are solved for a stacking fault probability of 0.2, the shift in h_3 is 0.012, for planes of the form $\{222\}$. When substituted into the equation

$$I_{\text{DIAMOND}} = 2 \left(1 + \cos \frac{\pi h_3}{2} \right) I_{\text{fcc}}$$

this shift will result in an intensity for planes of this form which is about 0.01 times the intensity of the brightest reflections in the crystal.

Reported intensities for planes of the form $\{222\}$ are from 0.01 to 0.10 times the intensity of the planes of form $\{111\}$ [20]. The corresponding shift in the Bragg angle when using molybdenum Ka radiation is only about ten minutes, a quantity which would be indistinguishable using photographic methods of x-ray diffraction.

This method predicts similar results for all planes for which $h+k+l = 4n+2$. However, as previously mentioned, a thorough search of the literature has revealed that the planes of the form $\{222\}$ are the only ones for which "forbidden" reflections have been recorded in diffraction studies of natural diamond, germanium, and silicon. Lonsdale has found, on the other hand, that diffraction maxima do occur from the $\{200\}$ and $\{420\}$ planes in synthetic diamonds grown by the General Electric Company [13].

A second discrepancy between the predicted and experimental results is the lack of any extra reflections in the diffraction patterns which would reveal the presence of a multiple unit cell, and hence give some evidence of the presence of twinning faults, as well as deformation faults.

Before attempting to find possible explanations for these discrepancies, the artificialities which exist in Paterson's model should be examined. The most glaring oversimplification is the assumption that stacking and growth faults occur on only one parallel set of close packed planes. In the actual case faulting can occur on any of the four sets of planes of form $\{111\}$ which are the close packed planes for crystals having the diamond or face-centered-cubic symmetries.

These artificialities, as well as the sort of mimetic effects which were suggested for the twinning of aluminum in the previous section, may contain the key to the discrepancies noted above. Lonsdale attributes the presence of the $\{420\}$ and $\{200\}$ reflections which she found in synthetic diamonds to the presence of islands of nickel or nickel-carbide on the order of 10,000 Å in extent, which she suggests are purposely precipitated in the growing process to act as seeds on

which the diamond lattice can nucleate [13]. The similarity of the lattice parameters of nickel (3.524 Å) and diamond (3.568 Å) would seem to make such seeding a feasible way to initiate the formation of diamonds in a synthetic process. Bundy, however, states that in his experiments at General Electric the use of seeding has not been necessary, since the diamonds nucleate spontaneously at the temperatures and pressures used [3].

It is therefore suggested that the origin of the {420} and {200} diffraction peaks in the synthetic diamonds may arise from the fact that the conditions of growth are different in the synthetic stones from those which occur in the natural formation of diamond within the earth. If the synthetic stones grow in a highly directional manner, the concentration of faults on one set of parallel close packed planes might be far larger than that occurring on the other sets. If this were the case, the conditions prevailing in the synthetic diamonds would much more nearly agree with the assumptions present in Paterson's model than do the conditions in natural diamonds, and would account for the presence of the {420} and {200} reflections from these crystals. This would suggest that there exists some mechanism which would cause further interference between reflections from the {420} and {200} planes when the concentrations of faulting on different sets of close packed planes are approximately equal, and the model does not approximate the real conditions as closely. Such a mechanism would, at the same time, have to allow the reflections from the {222} planes to be produced with little additional interference.

4. Experimental

This investigation has been carried out concurrently, and in the same laboratory, with research conducted by P. B. Hornbeck concerning the substructures formed by dislocation reactions in a single crystal of aluminum. There has been a free exchange of data and ideas in these investigations, and all data referred to in this paper concerning the presence of extra reflections in x-ray diffraction patterns from

single crystals of aluminum are the result of Hornbeck's work with the Buerger precession camera and of Randall's earlier work in this laboratory, using oscillating crystal methods [9, 19].

Although there are many reports in the literature of the presence of the {222} reflections in diffraction patterns from diamond crystals, there remained several points which were not sufficiently clear in the published material, and which seemed to dictate that first hand experimental data be gathered. Among these were questions as to whether all of the possible peaks of the form {222} appear in each diffraction pattern, whether other peaks with $h+k+l = 4n+2$ might also appear in some patterns, and if there was any other evidence of faulting, such as split peaks, extra peaks, or streaking. At one point in the course of the investigation, it also seemed possible that the reported "forbidden" reflections might not be from the {222} planes at all, but might, rather, be a reflection stemming from the existence of higher order twins in the diamond crystal. That is the reflections from some plane of a nine fold, or greater, unit cell might fall sufficiently close to the expected location of a {222} reflection to mislead an investigator who was not looking for this effect.

In order to investigate the possibility of such a misidentification, as well as to seek answers to the other questions listed above, a small diamond was obtained and mounted on a standard x-ray goniometer. The crystal was then oriented by means of Laue patterns so that the axis of rotation of the goniometer corresponded to the [110] axis of the diamond.

Oscillating crystal patterns were then recorded, using a flat plate cassette, but this did not prove to be a sufficiently accurate method of locating peaks in reciprocal space to resolve the doubts which existed concerning the correct interpretation of the "forbidden" reflections.

Consequently, it was decided to make use of the Weissenberg goniometer, which makes an unambiguous recording of the reciprocal space coordinates of each diffraction peak.

This method of recording x-ray diffraction patterns allows one level

or layer of reciprocal space intensity maxima to be recorded at a time, and if the zero level is chosen as the layer to be recorded, the so-called "central lines" of the layer appear as rows of spots on the film. The "central lines" are defined as those rows of reciprocal space points through which a straight line passing through the origin can be drawn. The rows of diffraction peaks corresponding to central lines appear as lines of spots on the film, each line having a slope of two when the axis of rotation is taken as the direction of the ordinate and the circumference of the cassette as the abscissa.

The peaks which will appear in a given level of reciprocal space must have Miller indices which satisfy the equation

$$n = hu + kv + lw$$

where h , k , and l are the Miller indices of the reciprocal space point; u , v , and w are the Miller indices of the axis of rotation; and n is the number of the layer being considered. For a crystal being rotated about its $[110]$ direction, the points which will appear on a zero layer pattern will be those which have indices $(h\bar{h}k)$ or $(\bar{h}hk)$. The appearance of these points in a diffraction pattern is subject, of course, to the restriction that the structure factor for that plane be non-zero.

The sequence of points $(1\bar{1}1)$, $(2\bar{2}2)$, $(3\bar{3}3)$, $(4\bar{4}4)$, $(5\bar{5}5)$, defines one of most densely occupied central lines on the zero layer when rotation is about the $[110]$ axis. There are, of course, four lines of this kind in the complete pattern of the layer. The points in these four lines can be represented by the Miller indices $(h\bar{h}h)$, $(\bar{h}hh)$, $(h\bar{h}\bar{h})$, and $(\bar{h}h\bar{h})$. Since no other central lines in the pattern pass through so many points, the appearance of these lines is unmistakable. A faint peak, lying on one of these lines and at the proper distance from the line made by the direct beam to correspond with the calculated Bragg angle for $\{222\}$ can only be that peak.

Several Weissenberg patterns were made of the diamond. In every case, where the exposure times were sufficiently long, the $\{222\}$ peaks appeared on each central line of points of the form (hhh) . No other

"forbidden" or otherwise unexplained peaks were noted in any of the patterns, nor were streaks or split peaks at all obvious in the patterns.

It should be noted, however, that due to the press of time and the lack of a monochromator which was adaptable to the Weissenberg goniometer, all of the patterns were made with only a filter to cut down on the continuous spectrum radiation and to remove the K_{β} characteristic wavelength. Monochromatic radiation, of course, would improve the resolution of faint peaks from the background. Judging from the experience of Hornbeck, it is necessary that single wavelengths be used in order to detect the very faint peaks which he has observed. Since most of the investigations reported in the literature also appear to have been made using filtered radiation, a careful study of diamond diffraction patterns using monochromatic radiation is still desirable.

5. Conclusions

The results reported here demonstrate a qualitative relationship between certain structural faults existing in crystals of the face-centered-cubic and diamond structures and the x-ray diffraction patterns which are obtained from these crystals.

The calculations of structure factors for triple and nine-fold unit cells resulting from first and second order twinning are in general agreement with observations which Leibovich, Randall, and Hornbeck have made on single crystals of aluminum and iron.

There can be little doubt that the shifting of peaks in reciprocal space, predicted by Paterson for faulted crystals will be accompanied by the appearance of non-zero intensities from those planes which meet the condition $h+k+l = 4n+2$ in crystals having the diamond structure. A stacking fault probability of 0.2 as predicted by the correlation between the observed intensities of (222) reflections and the models of Guentert and Paterson seems high for diamond. However, the effects of faulting on all possible sets of close packed planes have not been considered, and the development of a satisfactory mathematical model to describe this may suggest that lower probabilities will be required to produce the

observed effect, as well as explaining the absence of all planes of the form $h+k+l = 4n+2$, with the exception of the $\{222\}$ planes from the diffraction patterns of diamond. It should also be mentioned that there are other faults which could cause a departure of the crystal structure from the mathematically ideal description given by the Bravais lattices. Models should also be developed which describe such faults in order to determine the effects which they will have on diffraction patterns.

The development of these better mathematical models as well as more careful x-ray diffraction studies of macroscopically perfect crystals, using monochromatic radiation and long exposures should provide better agreement between experimental and theoretical results and add to the power of x-ray diffraction as a method of studying the departures of crystalline materials from mathematical perfection

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13. ABSTRACT

Calculations have been made in an attempt to predict the effects of microscopically find twinning and of stacking faults on the x-ray diffraction patterns which can be expected from single crystals of materials having the face-centered-cubic or diamond cubic structures. The existence and the effects on x-ray scattering of a coincidence lattice and multiple unit cell in twinned structures are discussed. Additional diffraction peaks are found to appear in diffraction patterns from twinned structures at reciprocal space positions which have non integer coordinates when referred to the reciprocal lattice of an untwinned crystal. These extra peaks lead to layer line spacings in rotating crystal patterns which are found to be proportional to 3^{-n} where n is the order of the twinning involved.

The extension of methods for determining the effects of random stacking and twinning faults on x-ray diffraction patterns, developed by Paterson and Guentert, is shown to predict non-zero intensities from those planes in faulted diamond crystals which have Miller indices such that $h+k+l = 4n+2$. It is suggested that this provides a partial explanation of the well known "forbidden" reflections from planes of the form $\{222\}$ in crystals having the diamond cubic structure.

The positions and intensities of the $\{222\}$ reflections from a small diamond have been confirmed using a Weissenberg goniometer.

14. KEY WORDS	LINK A		LINK B		LINK C	
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